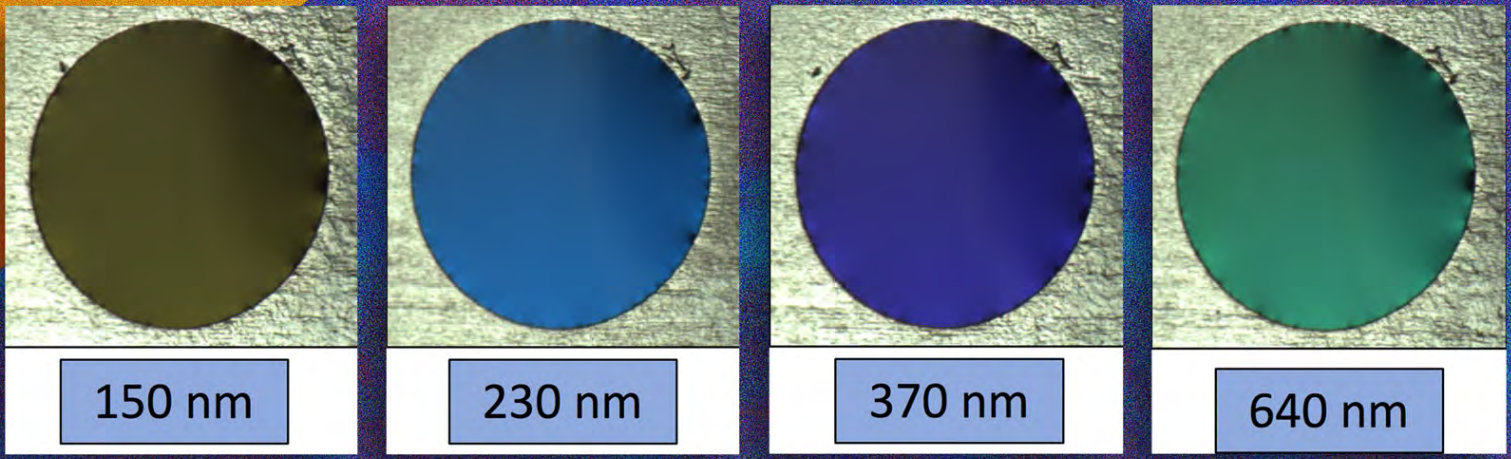
Workshop Report

Adaptive Sample Preparation and Target Fabrication for High-Throughput Materials Science

May 14–16, 2019
College Station, Texas

Sponsored by Los Alamos National Laboratory and the Texas A&M University System



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Workshop Report:
"Adaptive Sample Preparation and Target Fabrication for High-Throughput Materials Science"

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Executive Summary

High-repetition-rate brilliant and coherent light sources are significantly increasing the rate at which scientific experiments can be performed. An investment in transformative technologies to make samples of condensed matter could enable a paradigm shift for that field or open new exciting frontiers in high-energy density science (HEDS). This will especially be true for dynamic materials in extremes research or HEDS, where the repetition rate for placing samples into extreme environments is increasing and the samples or targets are irreversibly destroyed in each experiment. Research teams that are able to implement solutions to all aspects of the experimental process and enable a paradigm of high-throughput science will have the greatest success and impact.

There are two different directions for adaptive samples. One is research when the number of experiments can be greatly increased with increased volume, such as in high energy density science. The other is when flexibility and agility can aid Bayesian optimization computational methods and speed up the discovery process, as with materials science. Conducting a similar equation-of-state (EOS) experiment took three years on the OMEGA laser facility, compared to five days of shifts at the LCLS XFEL. New materials with improved properties have been found by guided optimization of experimental science. Adaptive sample preparation and target fabrication can create a tremendous return on scientific investment. High-throughput enabling precision science is also a desirable goal.

To address these issues, we sought a diverse set of innovative participants who had ideas of how to achieve this paradigm shift. We invited 42 researchers from a variety of disciplines and fields to attend a workshop in College Station, Texas, May 14–16, 2019. Many of the participants had never been in the same room before, and most found it very exciting to hear about new and different research. The goal was twofold: to define the challenges, i.e., "what

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Cover art credit: foreground, Douglass Schumacher (Ohio State University), ultrathin liquid crystals; background, Matthew Lee (Los Alamos National Laboratory), stereolithography printed spherical targets.

would we like to be able to do and why it is difficult to do so," and to describe the progress, approaches and capabilities, as well as the vision, "what we could do if we had more support."

The transformation in materials science enabled by high-throughput experimentation is so significant, it is difficult to know what technologies can best be applied. The workshop served as an environmental scan of current efforts in high-volume, flexible, and agile materials sample preparation and target fabrication. As such, it fostered collaborative interactions that take advantage of present advances. This report summarizes both our evaluation of the present environment and proposes ideas for future investment.

Participants at the workshop realized that we have a rare opportunity to combine three major initiatives: the Materials Genomics initiatives, the fields of artificial intelligence and big data science, as well as advanced manufacturing driven by science. This can come together in autonomous materials discovery systems, also known as materials acceleration platforms. It was agreed that if the issues and challenges of adaptive sample preparation could be solved, major advances could be made in multiple fields.

Particularly, growing needs by present and emerging user facilities were identified and discussed. Large-scale and possibly adaptive target fabrication is needed to enable high-repetition-rate experiments that are otherwise possible from these facilities. Depending on the type of experiment, either mass production of identical targets or fast prototyping will be needed. Metrology and characterization of samples add to the complexity of the problem. Other issues, including fratricide, debris, activation, and electromagnetic pulse, all have to be addressed.

The workshop produced some suggested short-term follow-on opportunities as well as some specific, planned collaborations. The importance, broad applicability of the solutions, and need for diverse technical contributions caused much discussion about the need for collaboratories. One idea was to expand LaserNETUS (see https://www.lasernetus.org) to provide for target availability and solutions for target supply for the user community.

To move forward, we would like to seek qualified sponsors willing to fund innovative projects that could be used at multiple facilities with a possible big payoff or return. To succeed in attracting sponsors, we will need to identify either:

- A key application, such as nuclear photonics / neutron radiography that requires high-volume and high-repetition rate;
- An important science campaign, such as an effort to generate a nearly complete set of opacity data or x-ray transition data that would drive enabling technology investment over the required several years; or
- A user facility open to innovative beamline proposals where autonomous systems could be developed with wide applicability.

The results of a well-conceived experiment on a specific materials target of interest could demonstrate the efficacy of the high-throughput autonomous approach. One particular idea is to encourage user facilities to provide preferential selection for the run-time of proposals that use a specific target delivery protocol.

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Introduction

High-repetition-rate brilliant and coherent light sources are significantly increasing the rate at which scientific experiments can be performed. In fields of molecular biology and chemistry, fluidic methods allow large numbers of samples to be prepared. Major investments in data science and machine learning are reducing the bottlenecks on data acquisition and analysis. A concomitant investment in transformative technologies to make condensed matter materials samples could enable a paradigm shift for that field as well. This will especially be true for dynamic materials in extremes research, where the repetition rate for placing samples into extreme environments is increasing and the samples or targets are irreversibly destroyed in each experiment. Research teams that are able to implement solutions for all aspects of the experimental process and enable a paradigm of high-throughput science will have the greatest success and impact.

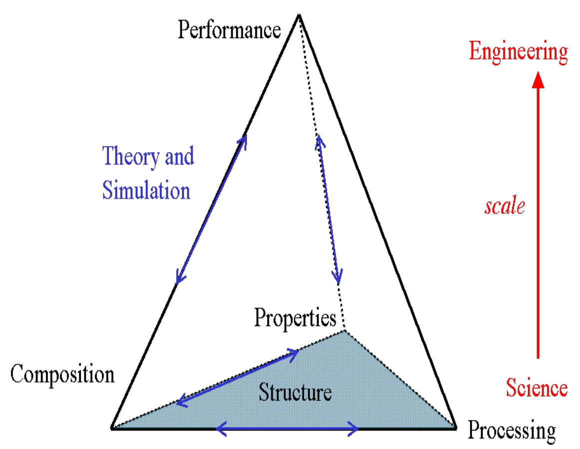
There are three qualities that technologies enabling the new paradigm would have:

1. Volume or numbers, i.e., the ability to make a large number of targets with controlled (and characterized) variability.
2. Flexibility, or the ability of the fabrication technology to vary design elements such as elements, thicknesses, locations of structures, and more. This was also called “variety.”

3. Agility, meaning the ability to implement a design change very quickly, perhaps in a day, an hour, or even several minutes.

We propose the term "adaptive" for technologies that could provide such volume, flexibility, and agility to scientific sample preparation.

There are two different directions for adaptive samples: research in which the number of experiments can be greatly increased with increased volume, such as in high-energy-density science (HEDS), and when flexibility and agility can aid Bayesian optimization computational methods and speed up the discovery process, as with materials science. A significant understanding of many basic physics issues in HEDS is still not readily available due to the single-shot nature of the larger facilities, where repetition is rare and parameter scans are costly. While smaller, materials-in-extremes facilities cannot achieve the integrated conditions required for achieving ignition, they can address some of those basic science issues. At such facilities, increased data rate, including agility to obtain such data, is becoming increasingly important (for example, rapid determination and validation of EOS or opacity data, etc.). These repetition-rated facilities can fill this gap in understanding very nicely as new diagnostic capabilities are added and new higher power optical lasers, pulsed power systems, or other material state drivers are developed.



The materials tetrahedron illustrates the relationships between process, structure (or composition), properties, and performance.

The other direction is in rapid materials discovery and process optimization. Central to scientific advance is the discovery and understanding of the relationships between processing-structure-properties-and-performance of materials, the PSPP linkages. More experimental data with variations in samples are needed. Here, adaptability needs flexibility and agility where the next sample to test or process to study can be quickly implemented when proposed by techniques such as Bayesian optimization, possibly driven autonomously by artificial intelligence tools. These materials or conditions can occur in HEDS, and similar adaptive technology is useful for those science campaigns. Similarly, many techniques described at the workshop used cheap computation to make up for expensive experiments in the optimization process; large and inexpensive volume with variability can help as well.

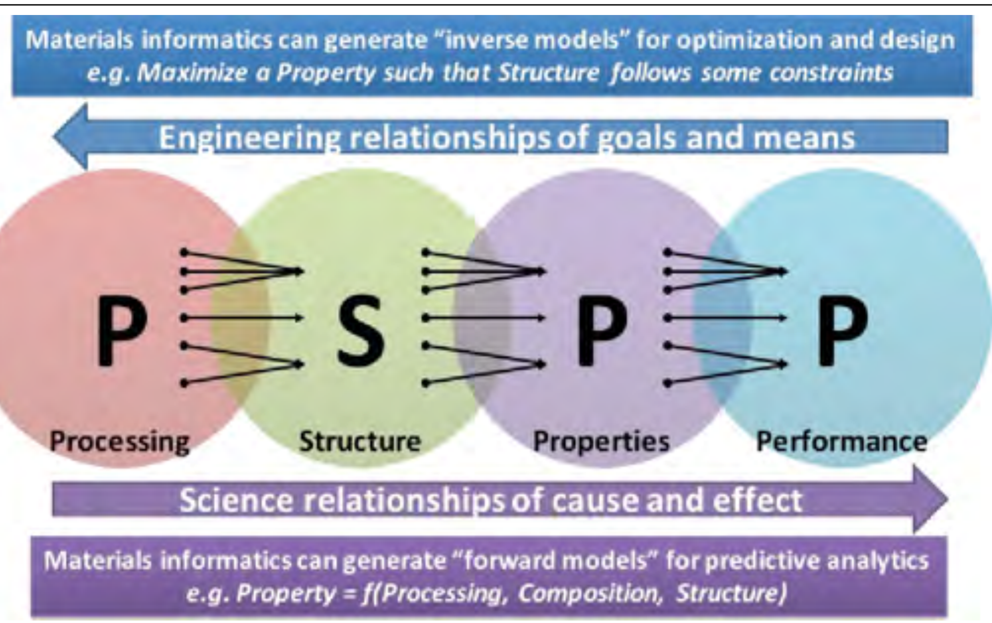
Targets for brilliant and coherent light sources are a new instance of a use case for high-throughput materials science. Not only do targets of different compositions have to be investigated, but also iso-compositional targets need to be synthesized by different processing schemes. Furthermore, given high repetition rates and the cost of performing experiments at such facilities, it would be advantageous to be able to perform synthesis and processing, and characterization of results in real time (order of seconds or minutes). Such experimentation can be carried out in AI-driven (autonomous) synthesis and characterization platforms, which can be collocated at the light source facilities.

To address these issues we sought a diverse set of innovative participants to a workshop who had ideas of how to achieve this paradigm shift. The transformation in materials science enabled by high-throughput experimentation is so significant, it is difficult to know what technologies can best be applied. The workshop performed an environmental scan of current efforts in high-volume, flexible, and agile materials sample preparation and target fabrication, as well as fostered collaborative interactions that can take advantage of present advances. This report summarizes both our evaluation of the present environment and proposes ideas for future investment.

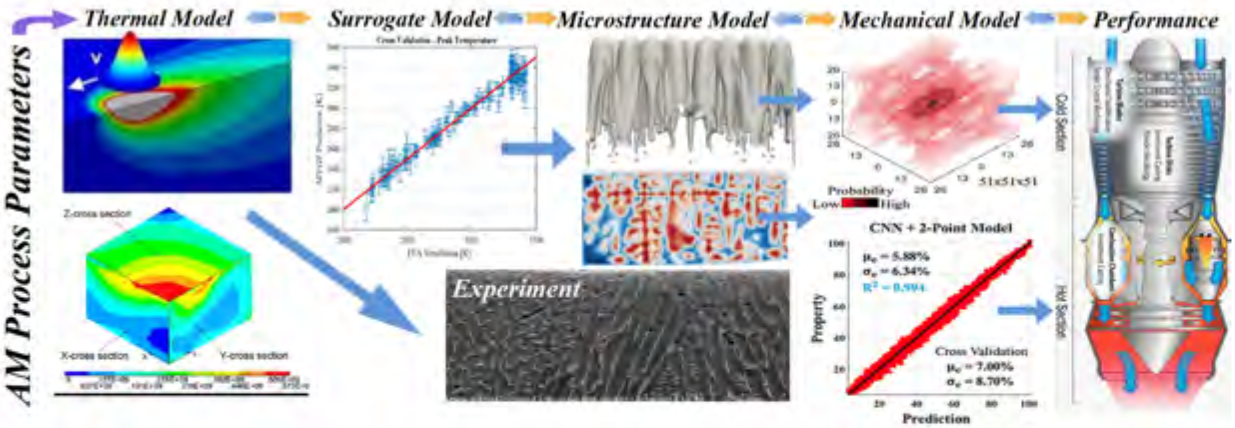
The Challenge

Developing Process-Structure-Property-Performance Linkages

The scientific need at the frontier of materials science is to address the process-structure-properties linkages that lead to materials' performance. Fabrication control of the atomic elements, stoichiometric composition, and material phase, as well as the ability to build in interfaces, longer-range (longer than molecular) structure, defects, and other controlled inhomogeneities, are required. While *in-situ* observation of fabrication processes will play a vital role in control of linkages between properties, process, and structure, individual samples, or targets, need to be made that can then be further subjected to environmental extremes and observed for their performance. Many samples will be identical, either to measure reproducibility and system uncertainties, or used while environmental conditions are varied. Most samples will want a controlled variation in some aspect of their fabrication. These



"Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science," APL Materials **4**, 053208 (2016); https://doi.org/10.1063/1.4946894, Ankit Agrawala and Alok Choudhary

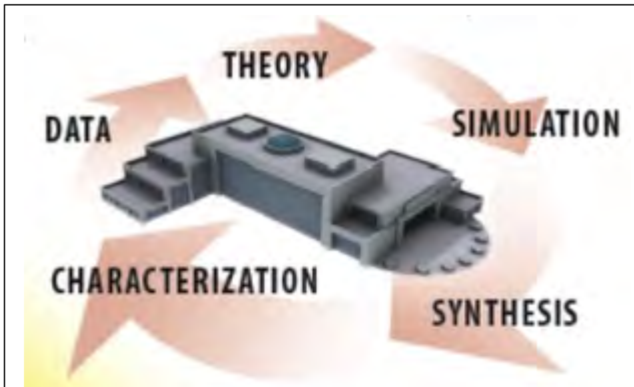


The multi-scale nature of the materials performance problem. From Mohamad Mahmoudi, Kubra Karayagiz, Luke Johnson, Raiyan Seede, Ibrahim Karaman, Raymundo Arroyave, and **Alaa Elwany**, "Calibration of hierarchical computer models with unobservable variables for metal additive manufacturing," International Journal of Machine Tool and Manufacture, Under Review (2019).

linkages develop at multiple scales, all of which are connected to determine device performance. As such, experiments are needed at all these scales.

Examples of the Challenges

- Current light sources are moving to optical laser pumping of materials' performance at ever-increasing rates. An experiment conducted every 10 seconds needs 3,000 targets to support an 8-hour shift. An experiment conducted 10 times per second needs 300,000.
- Sample size tends to increase with the energy of the environmental driver or the energy of the probe. As light sources move to higher energy and the drivers get more powerful the size and complexity of the targets will increase.
- Currently, experimental teams get campaigns on user facilities perhaps up to every 3 months. Given time for analysis of the previous campaign and design, a month is perhaps the total time available to provide samples for a campaign. But could these numbers of targets be made overnight for the next day's shift? And is it possible to have an assembly line of targets being



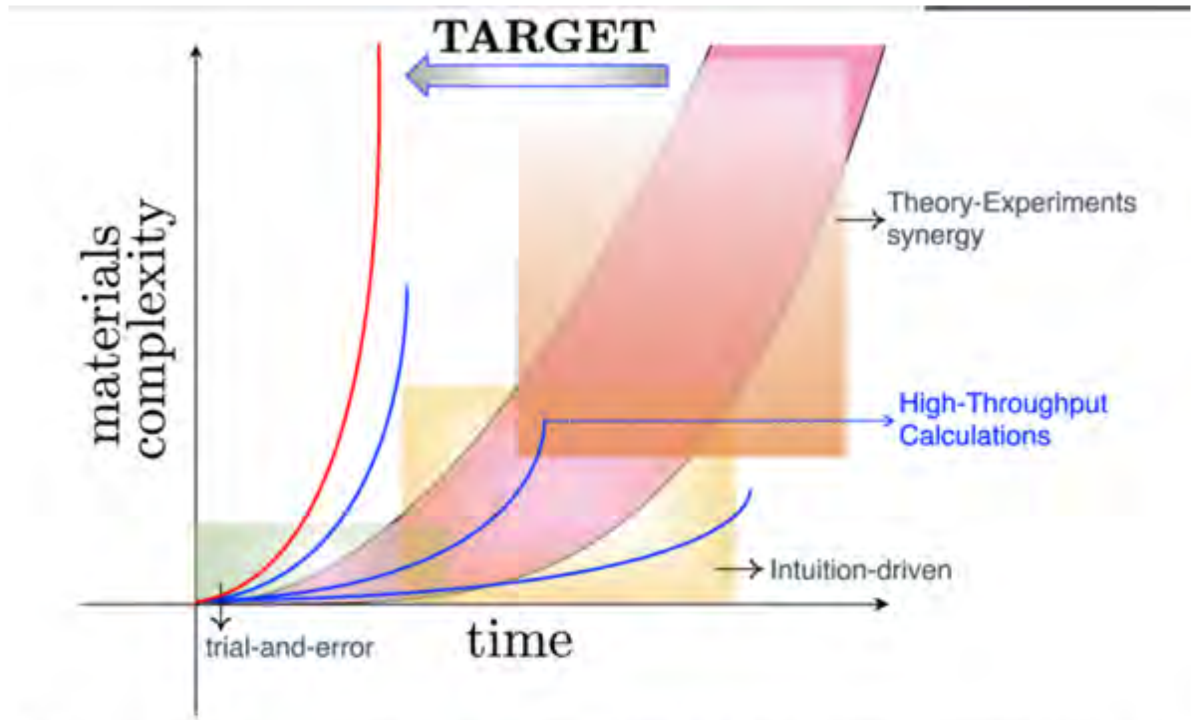
The experimental science co-design process illustrates that proceeding rapidly around this circle enables faster and better science. (The word "characterize" means to some the experimental result, rather than just the initial conditions for something dynamic.) (From **Cris Barnes)** fabricated with mere minutes between a design change request and a new sample series?

- And while thinking of going into the workshop had largely been devoted to dynamic experiments at x-ray free electron lasers, **Don Brown** made a strong case that the high average brightness of synchrotrons creates perhaps an even greater need for adaptive sample production.

Clockwise from upper left: beamline scientist, laser scientist, application engineer, theoretical physicist, data scientist. (Based on an idea from **Don Brown**.)

Major problems require big teams to collaborate; however, each member tends to bring different goals and success metrics to the project. Learning to work together is an issue. However, the diversity of the teams can be most helpful in finding new solutions to the challenges: “I was very naïve [at the beginning], so I could try something crazy.” (**Saniya LeBlanc**)

There have been a large number of workshops on high-throughput materials science in the last decade that recognize the importance of more experimental data to advance the field. At least 14 reports from a 10-year span have called for increased access to HTE methods and data (from **Martin Green**).



The trajectory for the discovery of new materials with increasing complexity as a function of time as we accelerate the process from trial and error to using high throughput calculations and statistical design methods to improve our ability to learn from existing data and make decisions for the next materials to test (TARGET)

"Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design," **Turab Lookman**, Prasanna V. Balachandran, Dezhen Xue & Ruihao Yuan, *npj Computational Materials*, **5**, Article number: 21 (2019)

Connections to the Materials Genome Initiative (MGI) and Artificial Intelligence: Bayesian Optimization

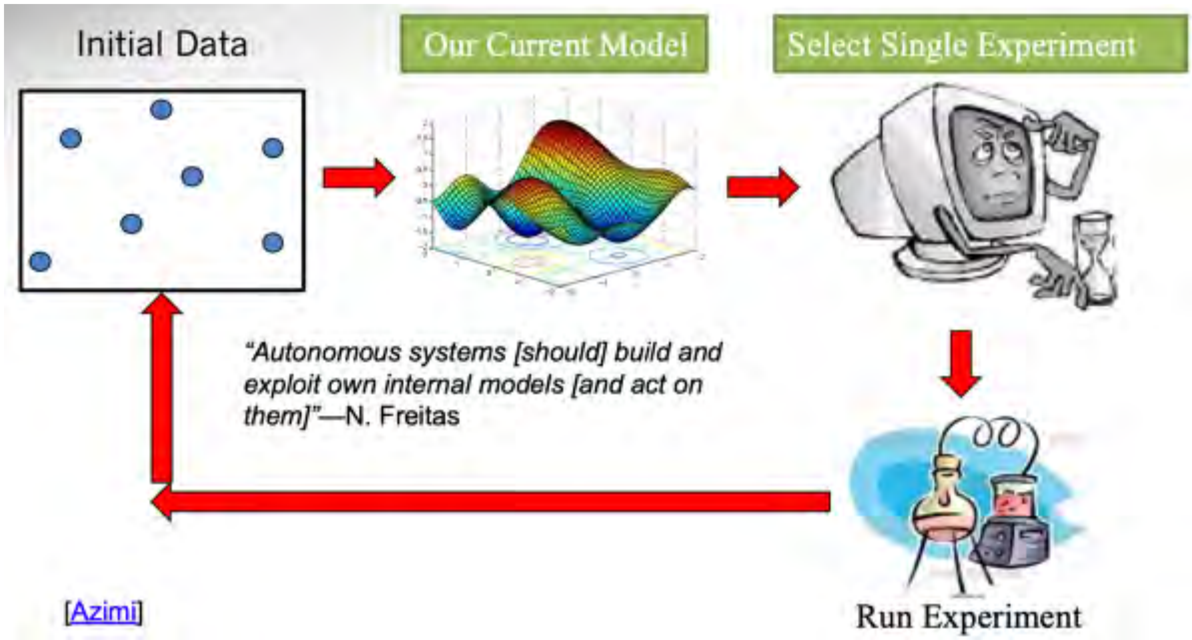
Participants at the workshop realized we have a rare opportunity to combine three major initiatives: Materials Genomics initiatives[1], artificial intelligence[2] and Big Data Science, and advanced manufacturing[3] driven by science. This can come together in Autonomous Materials Discovery systems (**Bukkapatnam**), also known as Materials Acceleration Platforms[4]. We

[1] "Materials Genome Initiative for Global Competitiveness," National Science and Technology Council, June 2011.

[2] "NATIONAL ARTIFICIAL INTELLIGENCE RESEARCH AND DEVELOPMENT STRATEGIC PLAN," National Science and Technology Council, October 2016. "Executive Order on Maintaining American Leadership in Artificial Intelligence," The White House, February 11, 2019.

[3] "STRATEGY FOR AMERICAN LEADERSHIP IN ADVANCED MANUFACTURING," National Science and Technology Council, October 2018.

[4] "MATERIALS ACCELERATION PLATFORM: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence," a Report of the Clean Energy Materials Innovation Challenge Expert Workshop, co-led by SENER, US DOE, and CIFAR, Mexico City, January 2018.



A simple overview of the Bayesian optimization process for materials discovery, that can lead to autonomous systems. (From **Raymundo Arroyave** (after Azimi).) After each iteration, the initial data becomes updated with additional knowledge from the experiment.

agreed that, if the issues and challenges of adaptive sample preparation could be solved, major advances could be made.

"The union of AI and materials science is emergent, i.e. it exhibits properties that neither AI nor materials science can exhibit outside alone. It will result in a sea-change in materials science practice, enabling a 100–10,000 times acceleration of materials discovery and process optimization, at reduced cost. … Complex materials are described by a high-dimensional space. We need to achieve maximum knowledge with minimum experimentation." (**Martin Green**)

There were a number of discussions (or presentations?) about machine learning, Bayesian optimization, and autonomous materials discovery systems. Many speakers seemed to approach the problem of materials discovery by asserting that if experiments are expensive, one can just throw lots of compute at the problem. There was an interesting – but inconclusive – discussion about the importance of real experimental ground truth in relation to getting a good answer. This involves verifying your prediction with an experimental result; thus, you need flexibility and agility in making sample types required by the machine learning algorithm. There was a lot of talk about optimizing the costs of the steps of the process versus the benefit that was being sought; this is an active field with many advances being made as research teams attack specific problems.

	Traditional AI Applications	Materials AI Applications
Data Volume	Big, dense (up to ~10^8 examples)	Small, sparse (~10^2 examples)
Prediction task	Accurately pattern-match	Want to find patterns as well as outliers
Domain knowledge	Not applicable (supervised)	Must be physics-aware (semi-supervised)
Uncertainty in data and models	Usually unimportant	Always important
Interpretability	Usually unimportant	Always important

Some of the important differences in applying AI algorithms to autonomous materials discovery. (From **Martin Green)**

Can making experiments cheaper beat such algorithms? There is a trade-off on volume versus adaptability – if we can make lots of sample frames, each with a wide variety of targets much greater than the possible number to shoot, we can then can pick and choose what samples on which to perform experiments. Having several target frames preloaded in the chamber, or readily added through a load lock system, combined with an automated mechanism for precisely placing them prevents an unnecessary venting cycle to replace the frame and can simplify the alignment between targets.

Needs by Present and Emerging Facilities

The availability of lasers with petawatt power and with 100's of Joules energy able to operate at 1-10 Hertz promise to dramatically increase the volume of available data, thus accelerating the scientific development. However, the efficient exploitation of these laser sources could be hindered by engineering issues intrinsic to high repetition rate operation (i.e., the increased production of debris) and by the lack of an appropriate target supply mechanism.

How some of us felt after hearing what can be discovered despite a dearth of experimental data.

Precision measurements for relevant physics at repetition rate

The high precision of an X-ray free electron laser (XFEL) facilitates measurements at a high repetition rate that will be relevant to larger systems. The bright X-rays of the XFEL can be focused to a micron-scale spot and be synchronized to the drivers, allowing probing microscopic conditions where other devices would require millimeter-sized targets. The key example of this is shock drive, where smaller focal spots and thinner targets can be profitably used to reach much higher shock pressures for a given laser energy because the pressures only need to be reached within the probe time. The limit here is the equilibration time or the shock formation. Similarly, hot dense plasmas existing in only a small area and for a very brief moment in time can be studied.

At LCLS, it will soon be possible to deliver up to 8 pulses per shot with a spacing of 360 picoseconds. This will allow dynamics within a driven target to be followed within a shot for a single target. Previously, such dynamics would have to be tracked over several shots with targets and laser conditions being close enough to one another to represent the same target. With multi-pulse capabilities, the constraints on target repeatability are relaxed. While not related to this workshop's issue of target fabrication, this capability is driving a strong need for up to 3-GigaHertz x-ray framing cameras.

Issues with petawatt- or kilojoules-scale interactions affecting target options

To succeed with a campaign at a materials-in-extremes facility, it is not just about fabrication or synthesis, but also characterization and alignment, EMP sensitivity of stages, debris mitigation, waste management, and many integrated issues that need to be solved as a system.

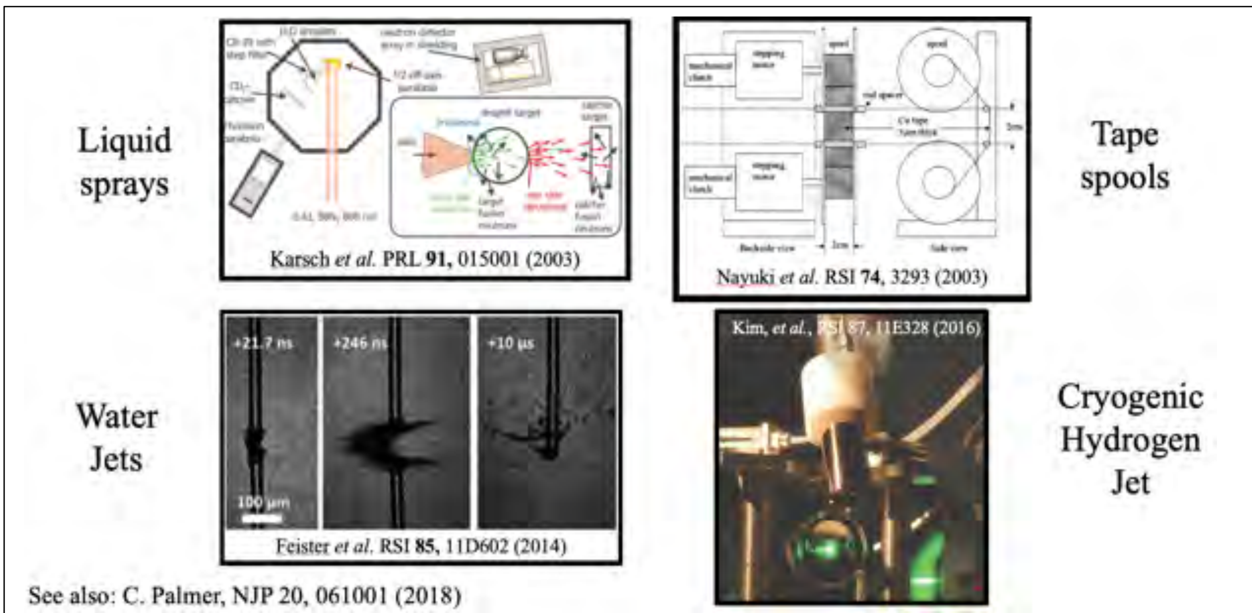
The petawatt /100s of Joules laser operation at high repetition rates requires technical solutions for a number of issues, including: target positioning and alignment; debris; activation, damage and thermal loads in the holder; damage to electronics (stages/controllers/detectors) due to electromagnetic pulses (for petawatt-class lasers); target back reflection and scatter (to be detected in real-time, together with possible damages in the optics, to immediately shut down the experiment and avoid damage propagation in the laser chain). Solutions to this technical problem could be developed in a wider collaboration between facilities; for example, tackling the single issues at different facilities with an incremental approach: automated irradiation at 0.1 Hertz first, then 1 Hertz, and finally 10 Hertz. Partial solutions are already available and European advanced laser facilities (HIBEF/HED at the European XFEL facility, ELI Pillars, CLF, CLPU, Apollon) are currently working towards the same goal and there may be an opportunity for strategic synergies with European facilities.

Solid targets for high-power/energy laser experiments are destroyed for each shot and their geometry and composition can be very different depending on the experiment (wires, ribbons, foils, multilayers, 3-D configurations, multi-target assemblies). They can by all means be considered expensive and sophisticated consumables. High repetition rate operation experiments will require large volumes of targets. Even the intermediate goal of 0.1 Hertz would require 720,000 samples per year, considering 2,000 operational hours per year. Current shot-on-demand campaigns require at least a few hundred – and up to 1,000 – samples with a cost of tens of thousands of dollars. Onsite target fabrication or modification is generally not available at facilities, therefore the only way for experimentalists to have some flexibility with target properties is to produce or purchase more targets than needed for the experiment, further increasing the number of required targets and the experiment costs.

Large scale and possibly adaptive target fabrication would therefore be needed to enable a high repetition rate irradiation. The development of a suitable target-support infrastructure should take into account the existing infrastructure and know-how, as well as focus on the development of complementary capabilities and competences that could then be replicated and exchanged.

Depending on the type of experiment (i.e., production of radiation beams versus exploratory studies), either mass production of identical targets or fast prototyping will be needed. Where large volumes of identical targets are required, processes developed for industrial mass production could be considered. MEMS techniques and lithographic capabilities could be of interest for targets with specific geometric requirements, such cone targets, arrays of pillars, gratings, and others. Coating techniques can be used for processing large areas of material to then be irradiated by rastering a foil or a cut into single targets. Rolling, thermal embossing, or gluing together with coating techniques could be considered to build a production/assembly chain for highly adaptive target fabrication (see **Alexander's** talk). A tradeoff between complexity and mass production could be needed. Rapid prototyping could be considered for exploratory studies that require tens of identical and complex targets. Possible techniques include two photon polymerization and additive manufacturing.

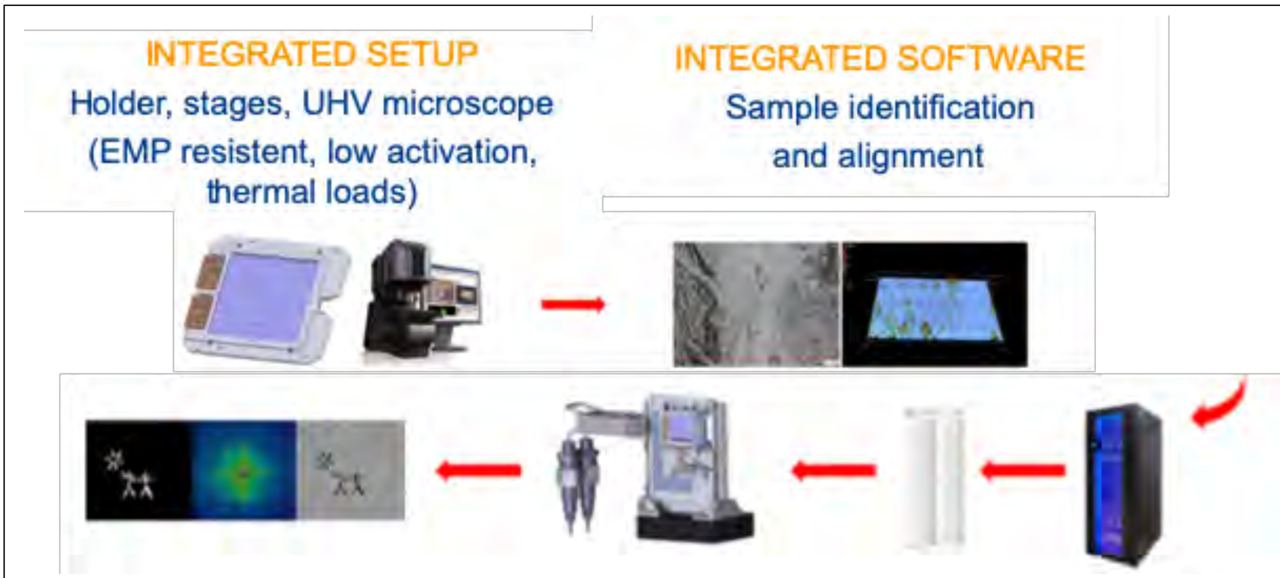
Metrology is also a fundamental aspect of the target fabrication process. Data interpretation require the best possible knowledge of laser and target parameters. Characterization of each single target, sometimes requested by principal investigators, is quite challenging for shot-on-demand experiments and contributes to a large fraction of the total fabrication costs (even



Examples of some high-throughput target systems. (From **Douglass Schumacher)** higher than 50 percent). Single-target characterization will not be an option for high-repetition rate experiments that will most likely rely on the characterization of the production process and of a few witness samples.

The platform for delivery of targets will reflect the repetition rate of a laser. In the case of few shots per day, a single target may be placed at laser focus and carefully manually aligned each time. In this case, the target can be loaded with an incorrect position and the orientation can be corrected prior to a shot. It may even be feasible to fully vent the interaction chamber between shots (the timescale is tens of minutes), manually accessing the center of the chamber to replace the target. In the case of the shot-per-minute scale repetition rate, it becomes infeasible to vent for every shot, so an array of targets may be shot, perhaps of an order of 100 or several hundred will be prepared ahead of time. In this case, the orientation should be identical or very nearly identical.

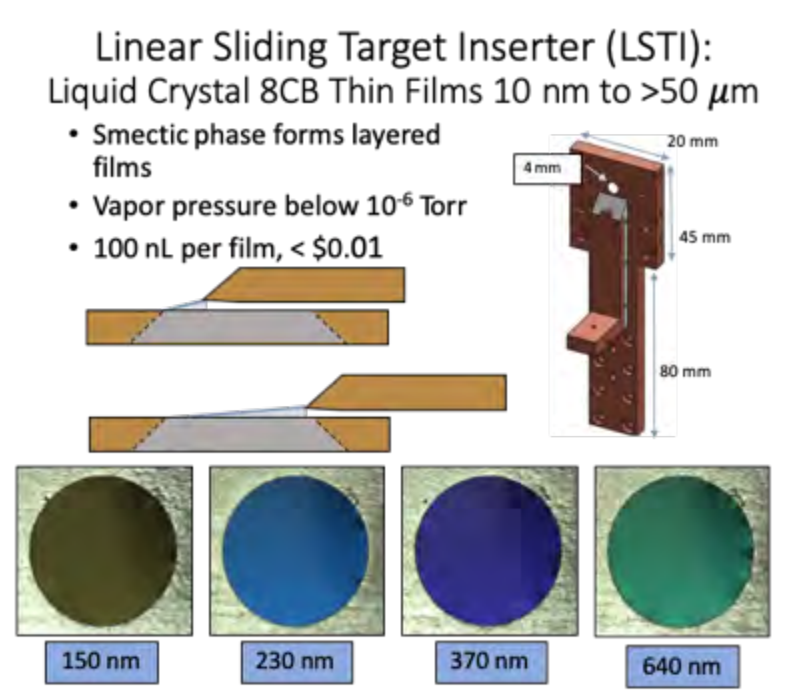
Moving to a Hertz or a multi-Hertz repetition rate will require a completely new approach for complex solid targets. The interaction chamber should be fitted to allow the replacement of targets without venting of the target chamber. One target concept is a miniature film reel platform that could be inserted robotically through a load-lock and brought to a target plane in a standard way. Such a platform could be standardized to some extent between different laser facilities and target manufacturing plants to deliver thousands of targets, potentially at Hertz or faster repetition rates. Manufacturing complex layered targets on such a target platform was presented as a prototype capability by **Alexander** of General Atomics. For petawatt- or kilojoules-scale laser experiments, the targets will need to be well separated and isolated enough from the reel to avoid damage at a level that would affect the loading mechanism.



From **Irene Prencipe,** originally from Carsten Deiter, European XFEL.

During this workshop, many other practical aspects of high-repetition-rate experiments at the petawatt and kilojoule level of laser matter interaction were presented. A few are summarized below:

- **Target fratricide:** Hundreds of joules of laser energy being delivered to a target generates expanding plasmas, shock waves, and extreme currents in the target and target mount, which can disturb or destroy neighboring material. Targets therefore need to be spaced by several millimeters and physical connections between them should involve as little material and as much space as practical.
- **Debris:** Any target that doesn't vaporize into a gas will tend to deposit on neighboring materials. A shot-per-hour petawatt laser facility shows visible coating of all chamber walls within a single experiment, consisting of perhaps 200 shots, or 20 seconds of 10 Hertz. Fortunately, the majority of the deposition is found to be the direct line of sight. Infrastructure allowing the important optics to be taken out of the line of sight, such as by ultra-thin plasma mirrors turning a corner, were presented at this conference and must be addressed.
- **Electromagnetic pulse and radiation:** Electronics must be robust against both a large-scale electromagnetic pulse from the displaced charge in plasma targets, as well as small-scale EMP caused by the ionizing particles impinging on electronics boards. Noise on detectors must also be addressed in algorithms.
- **Radiological activation:** Petawatt laser experiments can accumulate radiative activation of nearby materials, which will subsequently need to be handled appropriately. This can affect target loading mechanisms that are chosen.



The Linear Sliding Target Inserter concept presented by **Douglass Schumacher.**

Infrastructure capabilities such as drivers, diagnostics, and data science / reduction have received, and continue to receive, significant investment to enable faster learning in scientific areas (material science, material properties, and resulting physics) important to our sponsors. A great example that **Haefner** presented was the evolution of the HAPLS to SHARC to BAT laser systems that will be a game changer from a driver perspective. Another example is the application of machine learning (or AI) to more quickly generate decisions from the data that is being generated. As rep-rated facilities begin to more routinely operate at higher rates (0.1 → 1 → 10 → 100 Hertz, etc.), these issues become ever more important. However, an area of equal importance is the ability to make and field samples (targets), which has not received similar levels of investments. Without the appropriate fabrication characterization and fielding infrastructure, the advanced drivers will not realize their full potential. Past and current large national Inertial Confinement Fusion (ICF) and High Energy Density (HED) facilities (laser and others) have always prioritized getting the facility designed and constructed first with high-quality target fabrication and instrumentation development being secondary at best or an afterthought. The reason why this happens is completely understandable as large facilities are quite expensive and while managers and researchers have good intentions of developing target fabrication capabilities in parallel to facility design and construction, institutions have limited resources. As new high-repetition-rate HED and material science facilities come on line, the science community is quickly coming to the realization that the construction of high-quality high-throughput targets and samples will be the ultimate limitation for the understanding of current materials under extreme pressures and temperatures.

Single material targets

Single material sources will be the most readily prepared and will represent the first targets available for the highest repetition rate. The simplest targets are gas, followed by liquids and cryogenic liquified gases.

- Gas targets are routinely shot at the petawatt-level and Hertz-repetition rate for laser wakefield acceleration experiments.
- There is a straightforward path for certain types of liquid targets, either in the form of room temperature liquids, materials in solution, or cryogenic liquids such as hydrogen, argon, or deuterium. Prototypes of target delivery systems for such targets already exist[5] and serve as an example for the type of experiments that follow from the availability of high-repetition-rate targets.
- Microfluidics hold some promise in the creation of single-material or even multi-layered targets for any material that can be delivered in liquid form.
- We have also seen at this workshop the progress in the production of dynamically produced, repeatable, single material particle sources with fine control over particle size.
- Where thin CH targets are useful, we have seen the rapid creation of thin liquid crystal films through a low cost-per-target wiping technique. Such films were also shown to be very useful for other high-power laser infrastructure, such as plasma mirrors and possibly debris shields.

[5] "Efficient laser-driven proton acceleration from cylindrical and planar cryogenic hydrogen jets," Lieselotte Obst, Sebastian Göde, *et al.,* Nature Scientific Reports **7** (2017) 10248. "MeV proton acceleration at kHz repetition rate from ultra-intense laser liquid interaction," John T. Morrison *et al.,* New Journal of Physics **20** (2018) 022001.

Complex target bottleneck

The current limitations in the throughput and adaptability of target manufacturing are a major bottleneck to scientific discovery. Given the opportunity, scientists will design complex targets that enable multi-stage processes to be studied with the requirement of precise knowledge of target conditions.

- A multipart target for ion heating, in which the source of ions is necessarily a solid metal, and the sample to be heated by the ions is an arbitrary material. The source material may have tight tolerances on flatness, thickness, density, and purity. The sample material will need to be a pure sample of the material of interest, which may be a pure element or an alloy. Certain experimental requirements may also require mirror-like flatness of one surface as well as precise orientation of the surface. The two materials must be precisely spaced with micron-like accuracy over a distance of order a millimeter. While the area of interest on the target surface may be sub-millimeter, a high-energy petawatt pulse will destroy neighboring target material up to a centimeter away, particularly if the targets are connected.
- A multi-layer target for shock studies of a material of interest to be shot by a 100 joule- or kilojoule-scale laser will require, at minimum, an ablation layer of plastic, a material of interest, and a transparent optical quality window of appropriate material and optical quality to be layered with sub-millimeter thickness and micron-level accuracy. Additional material layers may also be required. Such targets may have a sub-millimeter interaction area, but the level of laser energy deposition generally requires targets to be disconnected and separated by several millimeters from one another.

Techniques of additive manufacturing are now progressing to a level where a wide variety of complex target types could be generated in a high volume and adaptive manner, given a basic framework. Such targets will require micron and sub-micron level precision, likely meaning that a combination of additive and subtractive techniques will be needed.

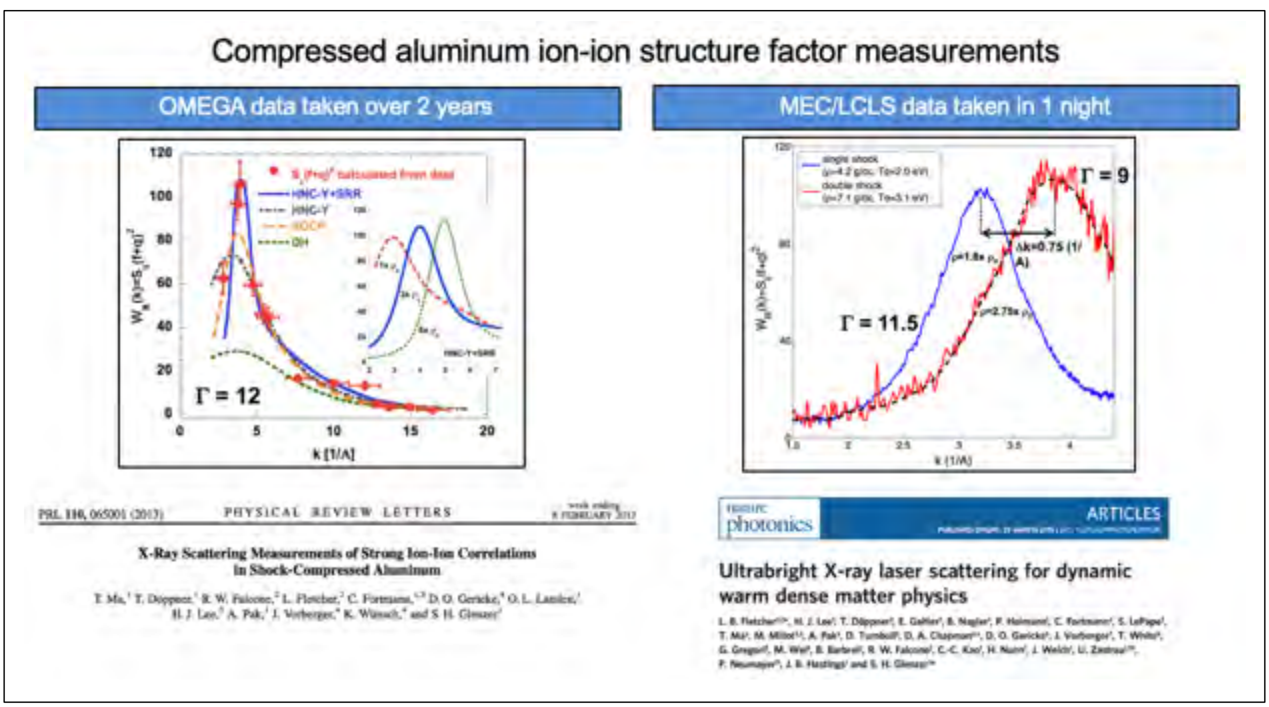
Complex precision targets may also be created with a refinement of techniques based on silicon wafer-based manufacturing processes, combining lithography, reactive ion etching, precise sputtering or deposition, polishing, subtractive manufacturing, and automated dicing and assembly. A single 4-inch wafer contains over 8,000 square millimeters in area, where a single target could be made from only a few square millimeters. Wafer manufacturing processes hold a high potential for automation. Examples of such nanofabrication such as those from the Office of Science’s nanotechnology centers were presented by **Quinn McCulloch** in his talk on the capabilities at the Center for Integrated Nanotechnologies (CINT) at the Sandia and Los Alamos Labs.

The Payoff: What Success Would Look Like

- "Hotter, denser, better, faster, and more opens many new exciting frontiers in HED science." (**Tammy Ma**)
- "As soon as you do something new, you see new unexpected things." (**Walter Gekelman**)
- "High throughput enables precision science." (**Constantine Haefner**, during his talk about the approach of high repetition rate optical lasers as drivers of extreme environmental conditions. Haefner's story about the NOVA petawatt and the many new processes it first discovered served as a great example of Gekelman's aforementioned sentiment.)

A good representative example of how high throughput science and target fabrication is having an exponential impact on the HED physics community is the work of **Tammy Ma** and others. Ma had spent more than 3 years conducting experiments on the Omega laser facility in Rochester, New York, performing an aluminum equation of state (EOS) experiment. With ~60 total shots and obtaining roughly 13 good data points, this was considered a highly successful experiment. Recently, the same experiment was conducted at the high-rep-rate LCLS facility in 5 days. And while the data was nicely reproduced, the economy of scale and value to get the same data from 3 years to 5 days is huge, opening real possibilities to other EOS experiments and general material science experiments.

High-repetition rate drivers of high pressure and HED conditions present the possibility of applying material discovery techniques to matter under extreme conditions. Two examples are the design of fusion materials, and the study of material resiliency under a dynamic load. In



both of these cases, small changes to alloy composition may be of interest in designing the best materials, but they must be delivered to a kilojoule or petawatt class system operating at a high repetition rate.

An experiment would start with an array of targets sparsely covering a parameter space, and the fabrication of new materials would then be guided by features in the output of the data. While full analysis of the data may take weeks or months, techniques of deep learning may be applied to suggest changes to materials as data is available.

Fusion liner

A strong case for petawatt -class rep-rated laser systems co-located with an XFEL is the study of fusion liners under particle bombardment. A laser driven ion source can generate extreme brightness of ions. The source may be a (relatively) straightforward cryogenic liquid droplet source of deuterium, methane or hydrogen, for example. A neutron source may be the same, with a semi-static converter. The alloy of interest would be placed in close proximity to the ion or neutron source and probed with 25 kiloelectron volts x-rays for wide- and small-angle x-ray scattering measurements of the dynamic response to radiation damage which is expected to be dramatic on the picosecond scale.[6] While the material of interest may or may not be destroyed on a shot-to-shot basis, a parameter scan of alloy composition informed by the x-ray measurements would be desirable.

Behavior under dynamic compression

Of particular interest are dynamically-compressed mesoscale materials. Targets for these studies require the multi-layer preparation of targets for laser-driven shocks, such as on a tape-drive-target delivery system, with output taking the form of a powder diffraction image. Experimentalists would define an objective based on a model for the connection between desirable material properties and the expected signal, and correct the model with the help of machine learning based on inferences from the data collected in real time. Examples of this at a low-repetition rate where data is costly was applied to NIF experiments by **Jim Gaffney.**

Collaboratories

An integrated, delocalized network of the synthesis and characterization tools is ideal for generating high-quality consistent data sets. It seems clear that having materials fabrication collaboratory associated with a user facility supporting multiple types of users is best. The European Cluster of Advanced Laser Light Sources (EUCALL) had a HIREP component that developed high-throughput target positioning systems and a target network, which identified strategic topics for collaborations and exploitation of the combined potential of partner infrastructure.[7] There are serious communication and culture issues between the interested

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[6] "Defect structures and statistics in overlapping cascade damage in fusion-relevant bcc metals," 511, 64–74 (2018).

[7] "Targets for high repetition rate laser facilities: needs, challenges and perspectives," I. Prencipe *et al.,* High Power Laser Science and Engineering, (2017), Vol. 5, e17, 31 pages, https://doi.org/10.1017/hpl.2017.18 See also

parties and their individual scientific goals. This is probably why we need teams and collaboration to integrate and achieve a common goal. However, there can be difficulties to bridging the users/facility community and the target fabrication community. A cultural issue can be intellectual property protection, which is a very important point for the target fabrication community. Also, often political goals and personal ambitions are very strong drivers, while the common scientific goal (the long-term development of the scientific/users' community) is not always compelling.

Collaboratory: A 1989 neologism (William A. Wulf, computer scientist at the University of Virginia): "…defined by…a 'center without walls,' in which the nation's researchers can perform their research without regard to physical location, interacting with colleagues, accessing instrumentation, sharing data and computational resources, …. accessing information in digital libraries."

How would a possible collaboration work?

1. Engineering high-repetition rate operation

Joint research activities would be beneficial. Each facility could be responsible for the development of a solution for a specific technical issue and lead the development in that field. Having clearly defined working groups, goals and timescales would help.

2. Adaptive target manufacturing

A possible collaboration could be initially focused on a class of targets, possibly for a specific science case or for a class of experiments. The choice should keep into account the complexity of the target and the availability of production, characterization, and assembly techniques already in use in the target fabrication community (possibly at one of the partner institutions) and/or at the industrial level. An example could be multi-layer targets for dynamic compression physics. The first step would be to develop a set of capabilities required for the production of such targets to be stationed at one of the facilities. For multi-layer targets this would include coating techniques (sputtering/PLD/CVD/thermal evaporation, Parylene coating, and others for flash coating, ablator, and sample layer), precision robotic assembly and gluing (for samples that cannot be deposited). Another possible example is the development of lithographic/MEMS techniques for micro/nano-structured targets. Each process should be well-characterized and described in a shared, public manner, so that a set of standard processes would be available at all times without need for R&D. Proposals requiring target R&D could be accepted for delayed experiments, giving access to R&D for target fabrication in the present experimental run (6 months) and to experiments in the next run. This approach could allow gradual expansion of the available capabilities, and offer know-how and familiarity with the process. Also, a gradual enlargement of the fabrication capabilities could include side projects for specific types of targets (for example aerogel and foams), possibly requiring a reduced initial investment. Development of complementary capabilities could be carried on in parallel at different facilities (either for the same target type or for different classes of targets for a larger scale

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http://www.targetsuppliers.com/ Workshop on "Targetry for high repetition rate laser-driven sources" (4th in Milan June 10–12, 2019).

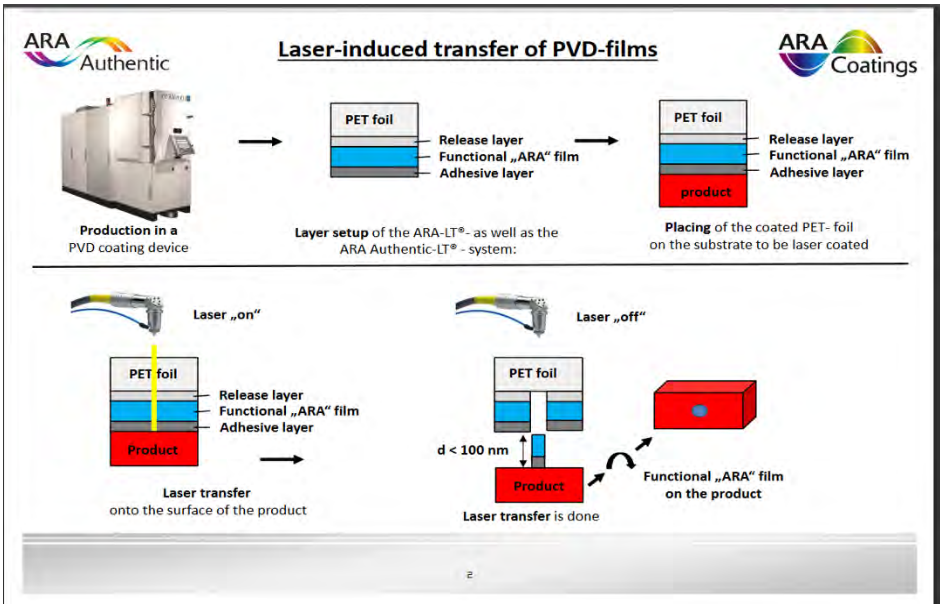
network). They could then be replicated at each partner facility (completely or partially, depending on needs and resources). The deposition and production of sets of graded targets could be beneficial for parameter space exploration, which could be the first step of an experimental campaign. Targets with optimized parameters could then be produced for the rest of the experimental campaign, provided that an efficient online data analysis system is available to support an informed decision. Campaign style experiments (multiple experimental groups with the same setup, but different targets) could be the best to this end: Each shift could be divided into shorter shifts of 2 to 4 hours long to be used for different experiments, giving time for data evaluation, decision making, and the fabrication of new targets. The reduction of target complexity in the design phase and the use of standard components and production steps, such as windows for VISAR measurements or membrane configuration on wafer, could reduce costs and the time required for target preparation.

Precision, low-volume manufacturing

Semiconductor foundries, which take orders from many different customers and produce computer chips of varying designs using the same basic manufacturing protocols, are examples of high-throughput, low-piece part (wafers) that can generate thousands of appropriately sized target-like components. However, lead time is long and each new design requires specific investment in specialized tooling. In the foundry case, the manufacturing processes have been highly developed and have appropriate process controls and process development that enable customized, precision fabrication. This level of investment is necessary across a wide variety of manufacturing science to enable needed technology options. We can learn from the foundries because targets are one of the few truly variable components of many HEDS and inertial fusion experimental designs.

Thus, we need investment in precision, low-volume manufacturing. Target fabrication is a relevant early test case. Precision means reproducible processes and low volume would still be considered high throughput for many target fabrication needs. Consider the simple case of multilayer foils. Currently, each foil is made in a series of steps depositing materials, usually metals by physical vapor deposition (PVD) and usually sputtering. An adaptive, flexible, and high-volume approach to make these foils could be enabled by using a laser-induced transfer (LIT) of PVD films. Several tapes of high-quality PVD materials at different thicknesses are prepared in advance. The schematic below shows the tape transfer process.

This process can be well-controlled and is commercially used. Multilayer structures of varying discrete thicknesses and compositions can be rapidly produced. Optimization of the release layer and input laser can control the kinetic energy of the transfer layer and obviate the need for an adhesion layer. Simple tests between sputtered and LIT films could be readily performed to validate performance under the extreme conditions required.



The technique will also allow ready incorporation of low and high Z metals, polymers, and ceramics (in arbitrary order), in contrast to current approaches, where the processing constraints, usually a high processing temperature, would limit the combinations of materials achievable. This technique can also be used to fabricate more complex hierarchical structures, where output tapes of precursor processes become input tapes for subsequent processing. In this way, as parts of the design become validated by the experiment, further optimization can be done even more quickly.

This capability could also be applied to investigations of corrosion studies where in-situ electrochemical cells could be fabricated with the materials to be tested (along the lines discussed by **Saniya LeBlanc**), allowing for more rapid optimization than currently done. Materials compatibility, including biocompatibility studies, would be able to be done much faster using LIT sample preparation, including the evaluation of sacrificial and barrier layers. Leveraging of the capability makes for an even less-risky investment.

Another example is in the development of the EUV light source that has enabled Moore's Law to continue. This liquid metal droplet source (target) took over a decade to develop and had a single purpose/application. It is a direct example of an HEDS-relevant, high-rep-rate target production at enabling operation up to 50 kiloHertz. However, the adaptability in the EUV light source is not in the target, but in the diagnostics and controls implemented within the system. This example directly speaks to the level of investment required over a sustained period of time to enable advancement in HEDS-relevant science.

These examples illustrate the benefits of implementing an autonomous materials discovery or materials acceleration platform in HEDS experiments. Because precision, low-volume manufacturing is currently an emerging topic in manufacturing engineering, there are great opportunities to both influence and leverage the technology development.

Innovative and Emerging Technologies

In this section, we describe some of the interesting and diverse presentations from the workshop and the important points they were making.

Again, during the course of this workshop with diverse participants, we saw some techniques better suited to materials or process discovery and some suited to providing a flexible volume of targets for a high-repetition rate. For the latter problem of achieving possible 1-Hertz operation at a dynamic user facility, **Alexander**'s presentation came close to describing a vision of how this might be achieved. The presentation did not, however, address concrete solutions and instead offered ideas to possibly pursue (which will not be cheap) with sufficient funding. **Prencipe** described the integrated approach attempted by the Europeans, following the solution used at LCLS as described by **Galtier**. This included the use of square frames holding multiple pre-made samples, which are rastered or scanned during an experimental operation. The system designed for the European XFEL[8] provides the possibility of substituting the frame without having to break vacuum, as was needed at LCLS. **Schumacher**'s presentation on hydrogenated liquid crystal thin-film devices suggested a catch-all solution for CH-based needs, both for targets as well as for plasma mirrors (which can improve or protect the laser optics) and for debris shields. Systems are being implemented at BELLA to be used at SCARLET (both are LaserNETUS facilities) as well as possibly in partnership with European facilities. **Bukkaptnum** described a low repetition-rate system with flexibility and in-situ correction with his study of 300-series austenitic steels. However, it is not clear if such techniques are sufficient for the specifications needed for the majority of HED experiments usually performed. In fact, it is not clear if any of the additive manufacturing techniques are really where they need to be for small, low-energy HED targets.

Autonomous Materials Discovery and Smart Hybrid Manufacturing

At the current nexus of materials genomics, big data science and AI, and science for manufacturing there were several presentations on accelerating the materials and discovery process and, in some cases, on making much of the cycle autonomous.

Generally, any application ends up in specific details. While the overall approach is generalizable,[9] it still requires a large investment to pivot to another problem. Some discussions (**Bukkapatnam, DeCost**) included single-cabinet tools integrated to an application. An alternative is to try for the modular or block model of a common input/output form that could be handed off in differing orders. **Alexander** talked about using cinema (film) technology to

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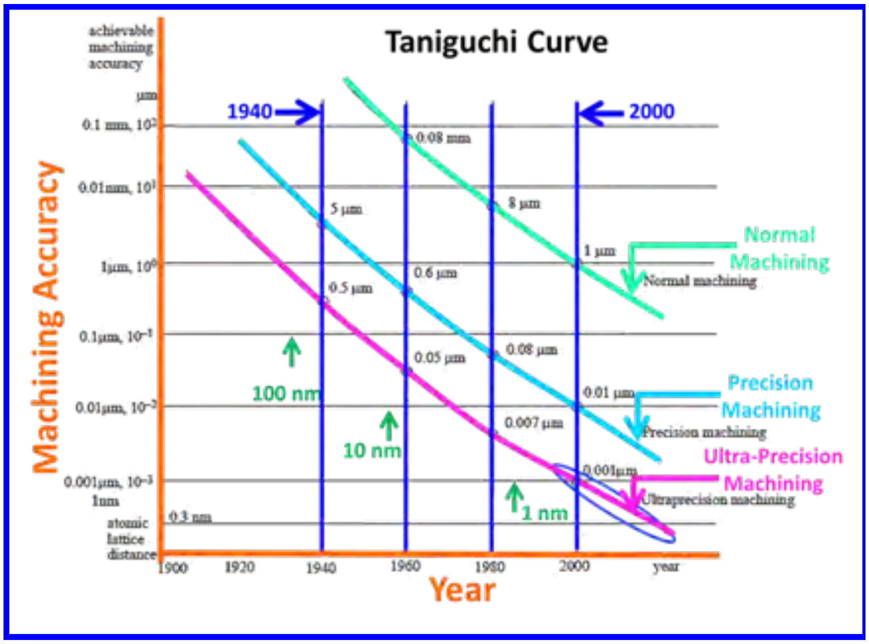
[8] https://www.eucall.eu/sites/sites_custom/site_eucall/content/e21597/e25317/e36136/EUCALL_WP6_HIREP_Deliverable_6_1_M13_31_10_2016.pdf?preview=preview

[9] Accelerating the discovery of materials for clean energy in the era of smart automation Daniel P. Tabor, Loïc M. Roch, Semion K. Saikin, Christoph Kreisbeck, Dennis Sheberla, Joseph H. Montoya, Shyam Dwaraknath, Muratahan Aykol, Carlos Ortiz, Hermann Tribukait, Carlos Amador-Bedolla, Christoph J. Brabec, Benji Maruyama, Kristin A. Persson & Alán Aspuru-Guzik, *Nature Reviews Materials* **3**, 5–20 (2018).



Precision in machining accuracy from various techniques has advanced significantly over many decades. Such improvements in precision and accuracy are required for smaller high-volume targets for many high-throughput user facilities.

frame each target, and feed into and out of various modules. and finally to experiment where alignment occurs. With 24-Hertz projection technology, one can get 13,533 frames on a reel.

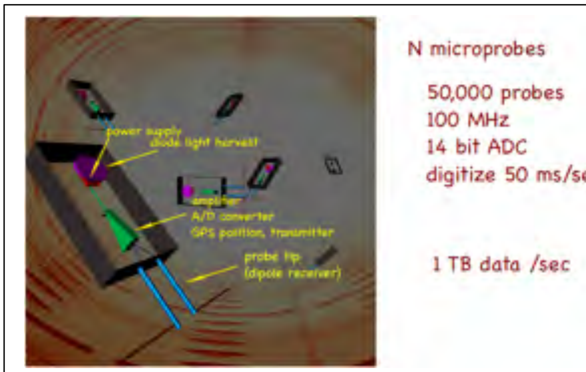
The machine learning used in this field tends to feature limited experimental data where deep learning techniques aren't applicable. **Xianing Qian**, in his study of MAX materials (M_2AX or M_3AX_2, where M is an early transition metal, A is a Group A element, and X is C or N) listed several challenges:

- Limited data (getting more requires time and funding);
- (Inaccurate models based on limited) scientific knowledge;
- Uncertainty (and noise in information);
- Interpretability (of results);
- Making the results verifiable and generalizable; and
- Simultaneously attempting multiple objectives.

This can be addressed for complicated multi-physics problems by using large ensembles of simulation results.

Other

For mesoscale light source science or HED, increasing resolution in fabrication techniques is important. In the last 40 years, accuracy specifications for the manufacturing processes in general have shrunk by 3 orders of magnitude. **Lee**, **Spadaccini** and others are using 2-photon polymerization techniques to get sub-micron resolution, but the fabrication rates are slow. Progress can be made with a closer connection with facilities and fielding issues, such as those discussed in the talk from **Galtier** at LCLS



High-volume fabrication could be applied to microprobes or embedded sensors, which results in vast quantities of data on the plasma or device. (**Walter Gekelman**) regarding the realities of fielding beyond fabrication. Fielding, by the way, is to be a subject on its own (as was in the case of IFE where target injection was separated from fabrication). There were several interesting discussions on possible fabrication techniques with some data on possible adaptability and agility, along with some numbers on throughput. Although a number of the talks were not necessarily geared toward the problem at hand (high throughput), some did address it directly. **Alexander's** presentation had specific examples from about 7 years of experience working on LCLS targets and tried to address some possible concrete solutions, but the myriad of distributed ideas will need substantial funding to pursue. It was hard to find a smaller set that would allow fabrication of all possible targets, or pick out a few for test cases. **Schumacher's** presentation suggested a catch-all solution for CH based needs, but that is not really the case. We need targets well in addition to thin CH. **Jaycox's** presentation begins to provide a vision for the future of HED targets. **Bukkapatnam** began to address the in-situ correction, but it is not clear if the technique is sufficient for the specifications needed for the majority of HED experiments usually performed. It took the steps towards instrumenting the fabrication unit with in situ diagnostics that can help with correction. **Jaycox's** presentation went more in-depth than others' in regards to high throughput and on-the-fly correction, including machine learning (ML) and AI integration into the process, though they are not necessarily being adaptive. **Spadaccini's** presentation showed the myriad of possible approaches with additive manufacturing (AM), but again, it was not clear how adaptable it is. In fact, it was not clear if any of the AM techniques are really where they need to be for these targets in terms of precision and resolution.

There were a variety of talks on use of AI (the Bayesian model, in particular) to tailor material properties to near-desired forms, but not necessarily in an either adaptive or agile or rapid manner for rep-rated experiments, although more rapid than traditional empirical approaches. In many cases, we do not need to design new materials. We need to be able to change the known materials on demand into shapes needed for the experiments. Hence, focusing the use of AI or machine learning to quickly resolve a fabrication problem would be quite interesting to pursue. **Jaycox**'s presentation offered an initial look into this, as mentioned above.
An example might be to address the adaptive rep-rated preparation of multi-layer foils to ~100-nanometer surface finish with no gaps. Further, on-demand changes to the materials may be good to consider as a demonstration. But such a demonstration should address needed underlying (transformative) capability development as current methods, such as physical vapor deposition or the like, already are being used and will not have the needed throughput.

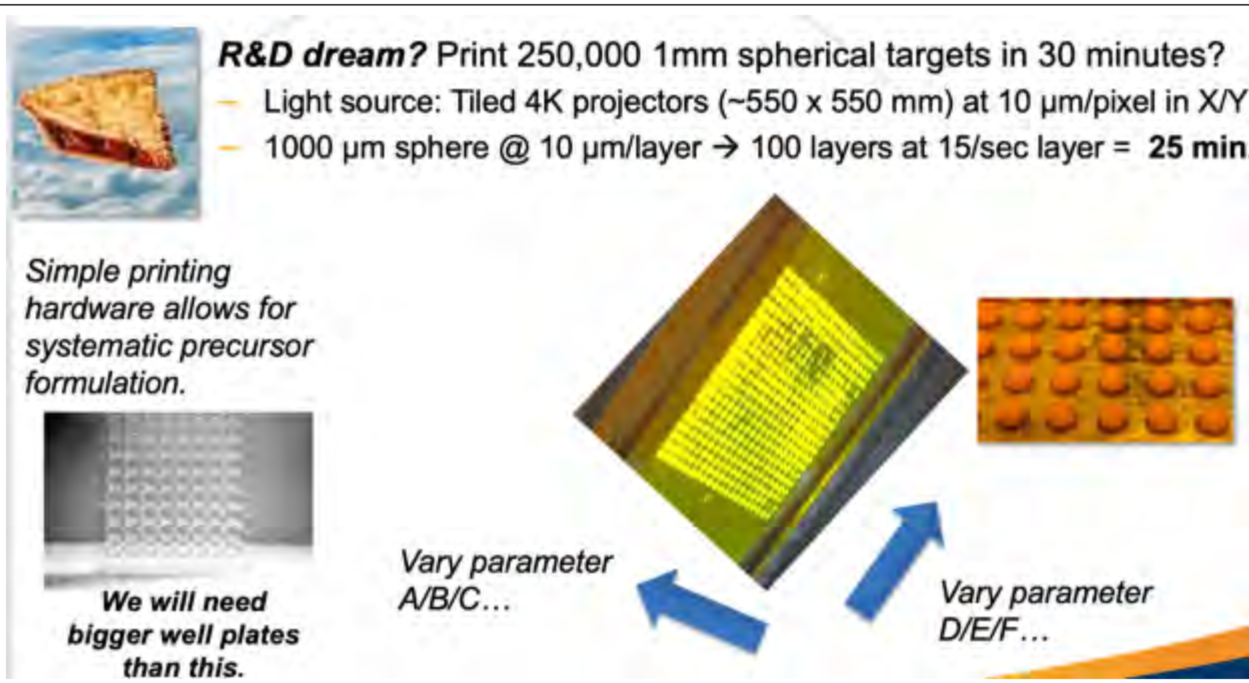
Comments on Path Forward

Sponsor Engagement

Most of the investment in sample preparation and target fabrication has been made as an institutional infrastructure investment or by facilities for their own needs. Asking the facilities themselves to fund the targets is difficult when they have their own issues of commissioning and operation. Simply trying to leverage infrastructure investment runs the risks of being too conservative and not being able to capitalize on emergent opportunities. Thus, we would like to seek qualified sponsors who might be willing to fund innovative projects that could be used at multiple facilities with a possible big payoff or return.

Qualified sponsors include:

- National Nuclear Science Administration (NNSA) defense programs and its Research Development Test & Evaluation directorate, NA-11, which funds both HEDS/inertial confinement fusion and materials science. It has made a huge investment in expensive facilities and needs to have a balanced investment to maximize the overall value and return in science.
- National Science Foundation (NSF), as perhaps an innovative beamline at the newly upgraded Cornell High Energy Synchrotron Source (CHESS).
- DOE's Office of Science, either through Basic Energy Sciences (BES) or Fusion Energy Sciences (FES) to help the APS-U synchrotron or the MEC beamline at LCLS get investment for a new revolutionary capability.
- Congressional initiative driven by universities may be possible, as some participants see this as a nexus of interest in big ideas.



A vision for high-volume yet flexible production of targets using stereo lithography techniques. (**Matt Lee)**

To succeed in attracting sponsors, we will need to identify either:

- A <u>key application,</u> such as nuclear photonics / neutron radiography that requires high-volume and high-repetition rate;
- An <u>important science campaign,</u> such as an effort to generate a nearly complete set of opacity data or x-ray transition data that would drive enabling technology investment over the required several years; or
- A <u>user facility</u> open to innovative beamline proposals where autonomous systems could be developed with wide applicability.

The results of a well-conceived experiment on a specific materials target of interest could demonstrate the efficacy of the high-throughput autonomous approach.

In addition to obtaining funding for a long-term program that could enable research on adaptive targets, a short-term collaboration of interested parties experienced in autonomous materials science from laboratories, institutes, and universities should be initiated.

Ideas

As expected, there are many gaps and hence opportunities. The intersection of Material Science with Manufacturing Science for the specific purposes of enabling adaptive sample preparation will continue to be a bottleneck to efficient utilization of significant investments made into highly capable rep-rated facilities. A lack of investment in sample and target fabrication will limit the potential progress of scientific advancement that these facilities offer.

Being first in the world in terms of these material science and HED fields requires theory, experimentation, and analysis. Experimental facilities are being developed, however a significant enabling capability that is lagging is the development of manufacturing and characterization sciences at the nano-to-meso scale precision. Investment is needed in manufacturing sciences that supports the other capability investments to keep pace with the idea generation and ability to execute even the most basic experiment, like gas puff or single foil experiments.

An investment into a new paradigm of target fabrication is needed, exploiting many of the exciting emerging technologies that are now becoming available. Leveraging additive manufacturing, machine learning, AI, deep learning and Big Data Science is already having an impact on how the target fabrication is done. While we are not completely there yet some of these techniques not only allow researchers to more cheaply build lots of targets, but also to ensure they have higher quality and better reproducibility.

There was a lot of thought about what type of adaptive, agile, and high-throughput fab should be done. A better focus on a particular problem at hand is quite useful; participation by an end-user input, such as shown in **Ma's** talk, can be very powerful if broadened to serve as justification for a particular effort. The diversity of a target's needs, based on physics data need, necessarily can make any endeavor quickly unwieldy. Therefore, having at least an initial consolidated-need statement can help guide determining fabrication capabilities required as well as identify gaps and challenges.

Observation: The present peer-review process of selecting proposals and assigning experimental time at rep-rated facilities hasn't historically taken in to account the commonality of experimental targets or target fabrication. For instance, if a rep-rated facility, such as LCLS MEC, decided for a six-month timeframe, preferential selection would be given to proposals that used a specific target delivery protocol, which would encourage both collaboration and infrastructure investment.

Investment in such an exciting new area of technology will advance our human intellectual capital as well. High-throughput projects will also involve training the next generation of stewards, not only in physics and design, but materials, fabrication and machine learning, and AI. In addition, this also enables fundamental science discovery in the area of dynamic materials and matter under extreme conditions. This is a natural progression of the Office of Science's investment in facilities such as LCLS or NNSA's investment at APS. Fabrication and ML/AI advancement at the university level, including a possible university collaboratory on target fabrication with labs in a steering or advisory role to enable technology research can be an efficient and key contributing factor to progress in capability development. University laser facilities are already organizing around LaserNETUS (see https://www.lasernetus.org/); target availability and solutions for target supply should be a key topic for this community.

Short-term follow-on opportunities from this workshop could include:

1. Better coordination between **Spaduccini** (LLNL) and **Lee** (LANL) related to advances in stereo lithography. The former can perform unprecedented systematic studies at a variety of length scales, while the latter can prepare chemical corollaries that will be manufacturable.
2. Develop strategies for replicates and deposition algorithms of particular material or process variations that, will allow results to be cross-checked between researchers.
3. Choose a model problem where Bayesian optimization can be combined with a target process optimization problem of general interest to illustrate exactly how the techniques are applied as well as the tricks and pitfalls that the community needs to be made aware.

Participants List

Alexander, Neil	General Atomics
Arroyave, Raymundo	Texas A&M University
Barnes, Cris	Los Alamos National Laboratory
Braun, Tom	Lawrence Livermore National Laboratory
Brown, Donald	Los Alamos National Laboratory
Bukkapatnam, Satish	Texas A&M University
Cardenas, Tana	Los Alamos National Laboratory
DeCost, Brian	National Institute of Standards and Technology
DeMleour, Michael	Texas A&M University
Dyer, Gilliss	SLAC National Accelerator Laboratory
Elwany, Alaa	Texas A&M University
Farrell, Michael	General Atomics
Gaffney, Jim	Lawrence Livermore National Laboratory
Galtier, Eric	SLAC National Accelerator Laboratory
Gekelman, Walter	University of California Los Angeles
Green, Martin	National Institute of Standards and Technology
Haefner, Constantin	Lawrence Livermore National Laboratory
Hamilton, Chris	Los Alamos National Laboratory
Hanson, Christina	Los Alamos National Laboratory
Herman, Matthew	Los Alamos National Laboratory
Herrmann, Hans	Los Alamos National Laboratory
Horwood, Corie	Lawrence Livermore National Lab
Iverson, Carl	Los Alamos National Laboratory
Jaycox, Adam	Lawrence Livermore National Laboratory
Karaman, Ibrahim	Texas A&M University- Department of Materials Science & Engineering
Kucheyev, Sergei	Lawrence Livermore National Laboratory
LeBlanc, Saniya	The George Washington University
Lee, Matthew	Los Alamos National Laboratory
Lookman, Turab	Los Alamos National Laboratory
Lopez-Bezanilla, Alejandro	Los Alamos National Lab
Ma, Tammy	Lawrence Livermore National Laboratory
Maestas, Lucy	Los Alamos National Laboratory
McCulloch, Quinn	Los Alamos National Laboratory
Muenchausen, Ross	Los Alamos National Laboratory
Nikroo, Abbas	Lawrence Livermore National Laboratory
Oertel, John	Los Alamos National Laboratory
Pokharel, Reeju	Los Alamos National Laboratory
Poole, Patrick	Lawrence Livermore National Laboratory
Prencipe, Irene	Helmholtz-Zentrum Dresden-Rossendorf
Qian, Xiaoning	Texas A&M University
Schumacher, Douglass	Ohio State University
Spadaccini, Christopher	Lawrence Livermore National Laboratory
Stach, Eric	University of Pennsylvania / Hummingbird Scientific
Yates, Kevin	Los Alamos National Laboratory

AGENDA

ADAPTIVE SAMPLE PREPARATION AND TARGET FABRICATION FOR HIGH-THROUGHPUT MATERIALS SCIENCE

Texas A&M University Hotel and Conference Center
College Station, Texas
May 14-16, 2019

MONDAY, MAY 13, 2019 – "Block T Bar," 2nd Floor Hotel

6:00 – 8:00 pm	*No-Host Meet and Greet / Early Registration*	

TUESDAY, MAY 14, 2019 – CORPS 1 MEETING ROOM

7:30 – 8:30	*Continental Breakfast and Registration – Outside of Corps 1 Meeting Room*	
8:30 – 8:45 am	Welcome and Charter	John Oertel, Los Alamos
8:45 – 9:15 am	The Revolution in Dynamic Materials Science	Cris Barnes, Los Alamos
DISCUSSION AND IDENTIFICATION OF CHALLENGES AND NEEDS	**SESSION CHAIR – Mike Farrell, General Atomics**	
9:15 – 9:45 am	The Materials Genome Initiative and the High-Throughput Experimental Materials Collaboratory	Martin Green, NIST
9:45 – 10:15 am	Beyond High-Throughput: Bayesian Optimization with Multiple Information Sources, under Budget	Raymundo Arroyave, TAMU
10:15 – 10:30 am	*Break and return to Corps 1 Meeting Room*	
10:30 – 11:00 am	(Machine learning and applying to high-throughput science)	Tammy Ma, LLNL
11:00 – 11:30 am	Building a Science Based Understanding of the Process/Structure/Property/Performance of Materials Fabricated with Advanced Manufacturing Techniques	Don Brown, LANL
11:30 – Noon	High Throughput Plasma Experiments	Walther Gekelman, UCLA

12:00 – 1:00 pm	*Networking Lunch, Brazos Restaurant (1st floor)*	*All*
All Participants Reconvene	***Corps 1 Meeting Room***	**SESSION CHAIR – Gillis Dyer, SLAC**
1:00 – 1:30 pm	Targets for pan-European Laser Facilities: the EuCALL target network for experiments	Irene Prencipe, HZDR
1:30 – 2:00 pm	Challenges of Target Delivery in Extreme Environments at FEL Facilities	Eric Galtier, SLAC
2:00 – 2:30 pm	(The revolution in rep-rated lasers and dynamic materials environments)	Constantin Haefner, LLNL
2:30 – 2:45 pm	*Break and return to Corps 1 Meeting Room*	
2:45 – 3:15 pm	~~Using Operando Methods to Combine Information from Multiple Data Streams~~	~~Eric Stach, University of Pennsylvania~~[10]
3:15 – 3:45 pm	Active Learning for Materials: Guiding Experiments Towards Targeted Properties	Turab Lookman, LANL
3:45 – 4:15 pm	(Challenges in WFO Space)	Ibrahim Karaman, TAMU
4:15 – 4:45 pm	*Break and return to Corps 1 Meeting Room*	
4:45 – 5:00 pm	Summary of Day 1	John Oertel, Los Alamos Cris Barnes, Los Alamos

[10] Dr. Stach unfortunately got sick and could not travel to this workshop.

ADAPTIVE SAMPLE PREPARTION AND TARGET FABRICATION FOR HIGH-THROUGHPUT MATERIALS SCIENCE

Texas A&M University Hotel and Conference Center
College Station, Texas
May 14-16, 2019

WEDNESDAY, MAY 15, 2019 – CORPS 1 MEETING ROOM

7:30 – 8:30	*Continental Breakfast and Registration – Outside of Corps 1 Meeting Room*	
8:30 – 8:45 am	Announcements	John Oertel, Los Alamos
DISCUSSION OF SOLUTIONS AND NEW TECHNOLOGIES **SESSION CHAIR – Abbas Nikroo, LLNL**		
8:45 – 9:15 am	Smart Manufacturing Platforms for Autonomous Materials Discovery: Identification of Surface Microstructure from Acoustic Emission Analysis	Satish Bukkapatnam, TAMU
9:15 – 9:45 am	Bayesian Learning and Experimental Design for Materials Discovery	Xiaoning Qian, TAMU
9:45 – 10:15 am	Autonomous Scanning Droplet Cell for On-Demand Alloy Electrodeposition and Characterization	Brian DeCost, NIST
10:15 – 10:30 am	*Break and return to Corps 1 Meeting Room*	
10:30 – 11:00 am	Ultrathin Targets Based on Liquid-Crystals for High-Repetition Rate, High-Power Lasers for Ion Acceleration and Neutron Generation	Douglass Schumacher, Ohio State University
11:00 – 11:30 am	High Throughput Solid Target Fabrication and Fielding	Neil Alexander, General Atomics
11:30 – Noon	"Upgrading" Stereolithography for Engineered Foams: Hierarchical Structures & Programmable Chemistry	Matt Lee, LANL
12:00 – 1:00 pm	*Networking Lunch, Brazos Restaurant (1st floor)*	*All*
All Participants Reconvene ***Corps 1 Meeting Room*** **SESSION CHAIR — Raymundo Arroyave, TAMU**		
1:00 – 1:30 pm	Additive Micro- and Nanomanufacturing: Materials and New Methods	Chris Spadaccini, LLNL

1:30 – 2:00 pm	Ultrafast Laser-Based Rapid Prototyping and Other CINT Sample Preparation Capabilities	Quinn McCulloch, LANL
2:00 – 2:30 pm	Rapid Melting and Solidification of Semiconductor Materials during Laser Additive Manufacturing	Saniya LeBlanc, GWU
2:30 – 2:45 pm	*Break and return to Corps 1 Meeting Room*	
2:45 – 3:15 pm	Machine-learned Predictive Models: Rapidly Incorporating Experimental Data to Improve Simulation Predictions	Jim Gaffney, LLNL
3:15 – 3:45 pm	(Solutions and Techniques Briefing)	Alaa Elwany, TAMU
3:45 – 4:15 pm	(Additive manufacturing and machine learning)	Adam Jaycox, LLNL
4:15 – 4:45 pm	*Break and return to Corps 1 Meeting Room*	
4:45 – 5:00	Wrap-up and Summary of Conference	John Oertel, Los Alamos Cris Barnes, Los Alamos

ADAPTIVE SAMPLE PREPARTION AND TARGET FABRICATION TO ENABLE HIGH-THROUGHPUT MATERIALS SCIENCE

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THURSDAY, MAY 16, 2019 – HONOR BOARD ROOM

7:30 – 8:30 am	*Continental Breakfast – Outside of Corps 1 Meeting Room*	
8:30 – Noon	Discussion and Report Writing	Organizing Committee and Session Chairs
12:00 – 1:00 pm	*Working Lunch, Honor Board Room*	*Organizing Committee*
1:00 – 2:00 pm	Summary of Draft Report; Establish Deadlines for Final Report	Organizing Committee